Cluster-based characterization of multi-dimensional tropospheric ozone variability in coastal regions: an analysis of lidar measurements and model results

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AMS 2022 Oral Presentation

Session: Addressing Air Quality Challenges at Urban–Land–Water Interfaces during Recent Field Studies. Part I

UNIVERSITY of HOUSTON

EARTH AND ATMOSPHERIC SCIENCES

Goal: Use multi-dimensional lidar measurements from campaigns to evaluate simulated coastal O_3 events

-- Directly address difficulties of measuring, modeling, & forecasting the large variability of O_3 in coastal environments

-- Use 2-D high temporal & fine resolution lidar measurements to help elucidate gaps within current air quality models

-- Complete observing system (surface land & water observations, model simulations)

=> a formidable tool for evaluating air pollution in coastal regions

-- Evaluate the ability of hourly temporal O_3 measurements & improve the abilities to simulate coastal O_3 concentrations

NASA Air quality campaigns

- 3 recent air quality campaigns:
  - OWLETS 1 (O_3 Water-Land Environmental Transition Study): July 5 - August 3, 2017
  - OWLETS 2: June 6 - July 6, 2018
  - LISTOS (Long Island Sound Tropospheric O_3 Study): July 12 - August 29, 2018

- Suite of detailed airborne & ground measurements measurements (e.g. ozonesonde, aerosol profiling - ground-based ceilometers, Pandora spectrometer, POM, etc.)

- Two <u>TOLNet lidars</u> used:
  - NASA Goddard Space Flight Center (GSFC) Tropospheric Ozone (TROPOZ) Differential Absorption Lidar (DIAL; Sullivan et al. 2014, 2015a)
  - NASA LaRC Mobile Ozone Lidar (LMOL; De Young et al. 2017; Farris et al. 2018)

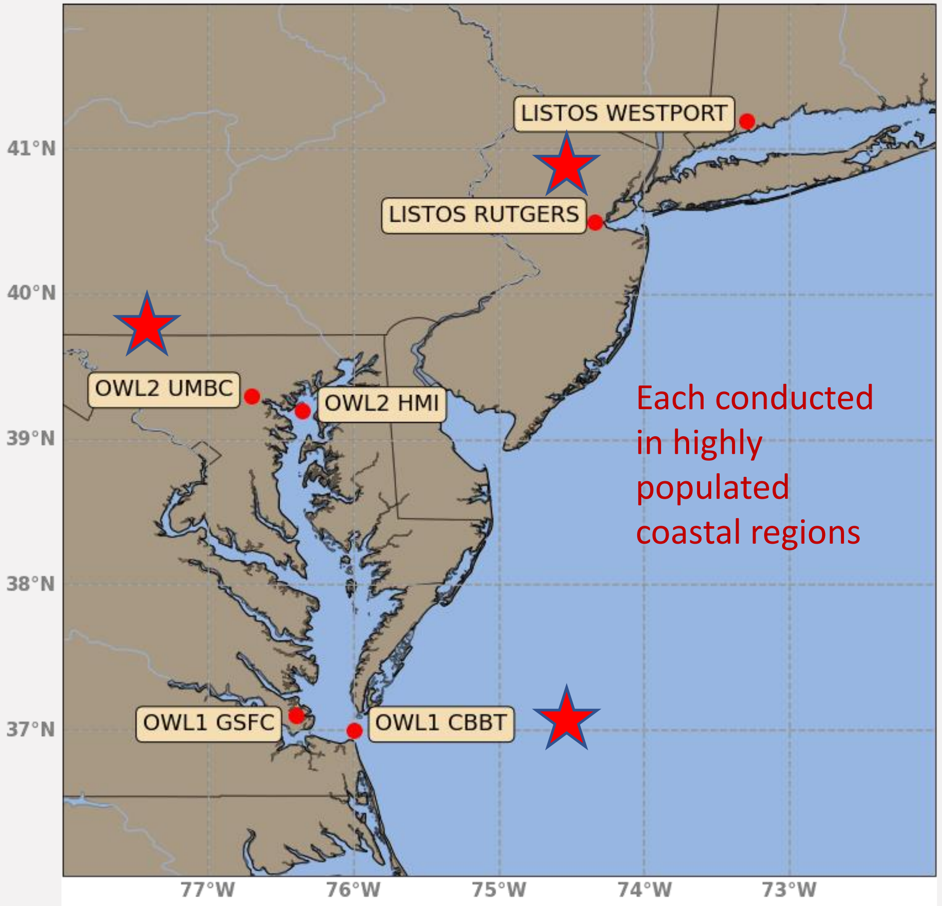
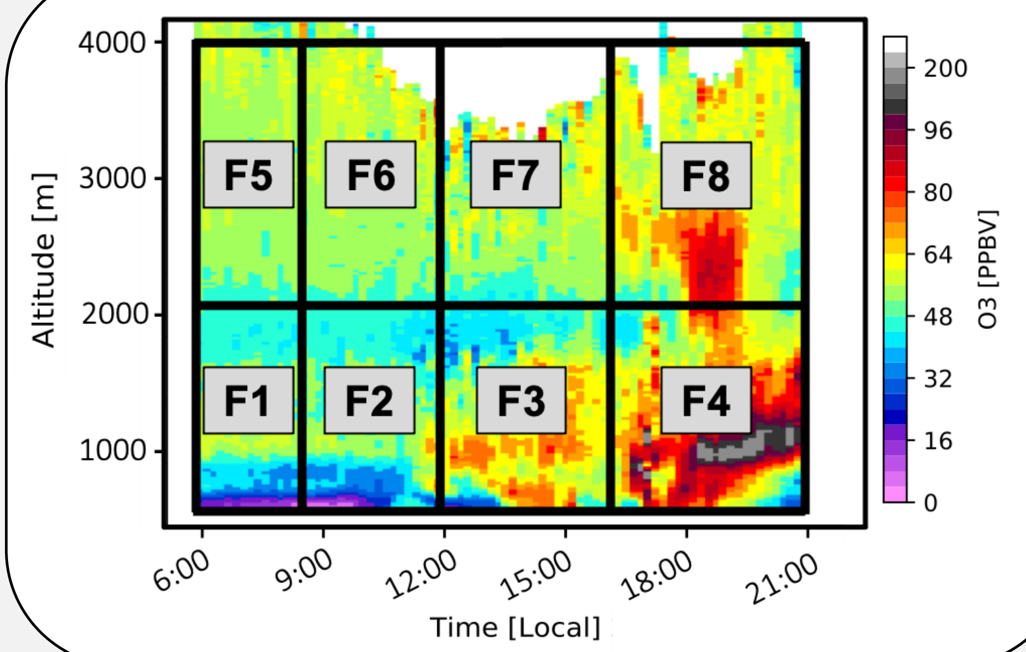


Figure 3. Inset map of Chesapeake Bay airshed in Maryland, VA and Long Island Sound in NY with 6 lidar monitoring locations used for OWLETS-1, OWLETS-2, & LISTOS (highlighted & labeled).

91 individual 2-D profile curtains used from both lidars:
- **26** from OWLETS-1,
- **28** from OWLETS-2,
- **37** from LISTOS
- https://www-air.larc.nasa.gov/index.html

Characterizing O_3 profile curtains



- Color coding *(left)* shows a typical O_3 profile taken from a lidar instrument
  - *August 6, 2018; LMOL at Westport, CT; LISTOS Campaign*
- Developed clustering method for characterizing 2-D O_3 curtain profiles from lidar measurements
- Constrained by the goal of evaluating lower level tropospheric O_3 limitations of the lidar measurements

- Split profiles (91 total profiles) into "slabs" based on **altitude** & **time**
  - F1 – F8 *(above)* indicate input feature ranges
- Calculated average features implemented into K-Means Clustering algorithm

<u>Features:</u>

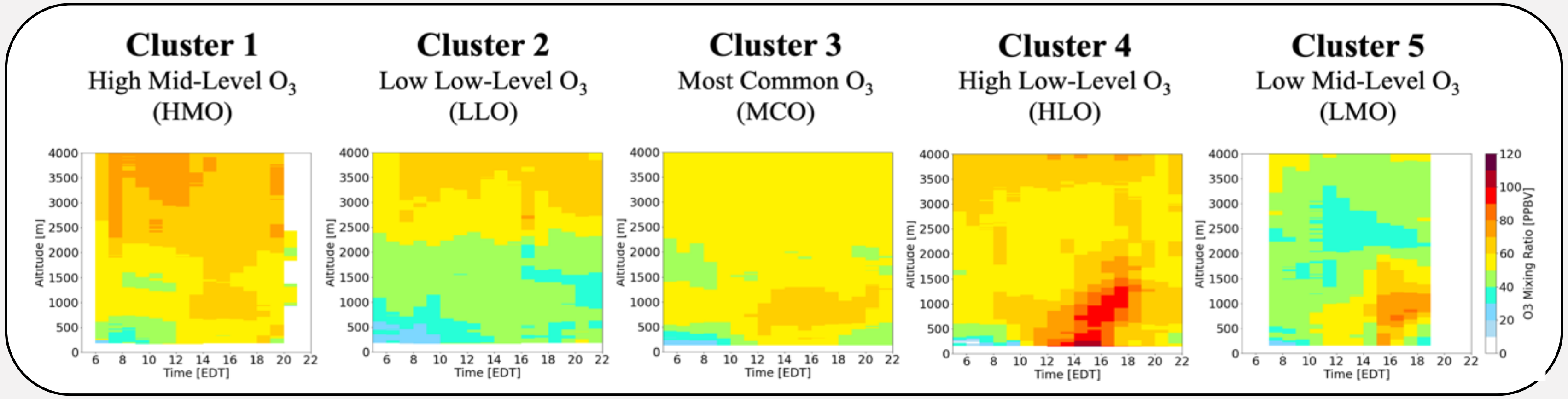
▻ **Altitude 2 sectors:**	▻ **Time 4 sectors:**
• 0 – 2000 m (low-level)	• 6:00 – 8:00
	• 8:00 – 12:00
• 2000 – 4000 m (mid-level)	• 12:00 – 16:00
	• 16:00 – 21:00

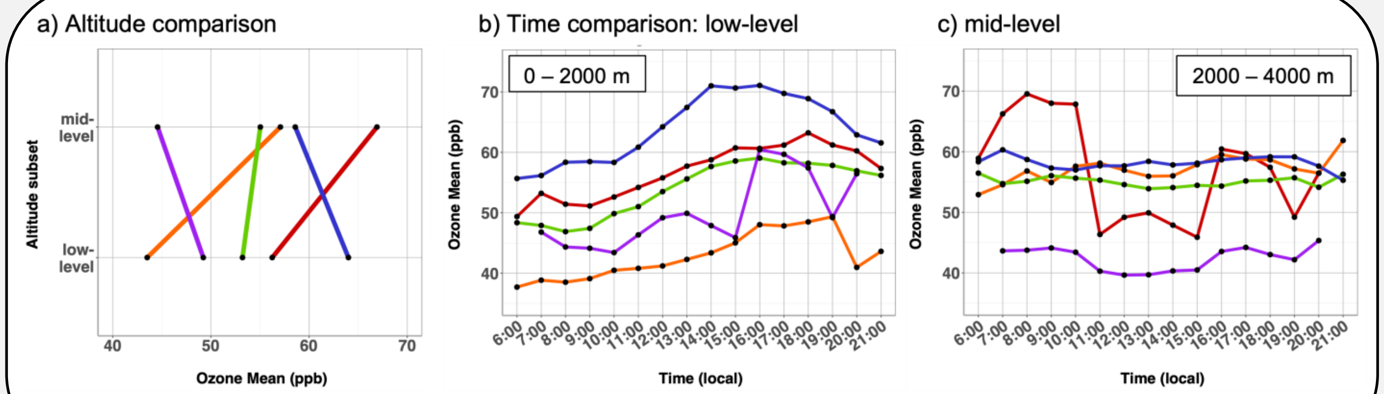
Clustering O_3 profiles

Cluster #	a) No. of profiles	b) O_3 Max (ppb)	c) O_3 Min (ppb)	d) T (°F)	e) WS (m s^{-1})
1	25	86.50	42.17	73.80	1.51
2	14	72.77	28.85	71.42	1.62
3	27	86.64	34.18	77.34	1.30
4	18	97.77	44.08	77.79	1.24
5	5	67.70	29.07	74.93	1.51

Fig. Cluster statistics

- Mean lidar O_3 vertical profiles for each of the clusters



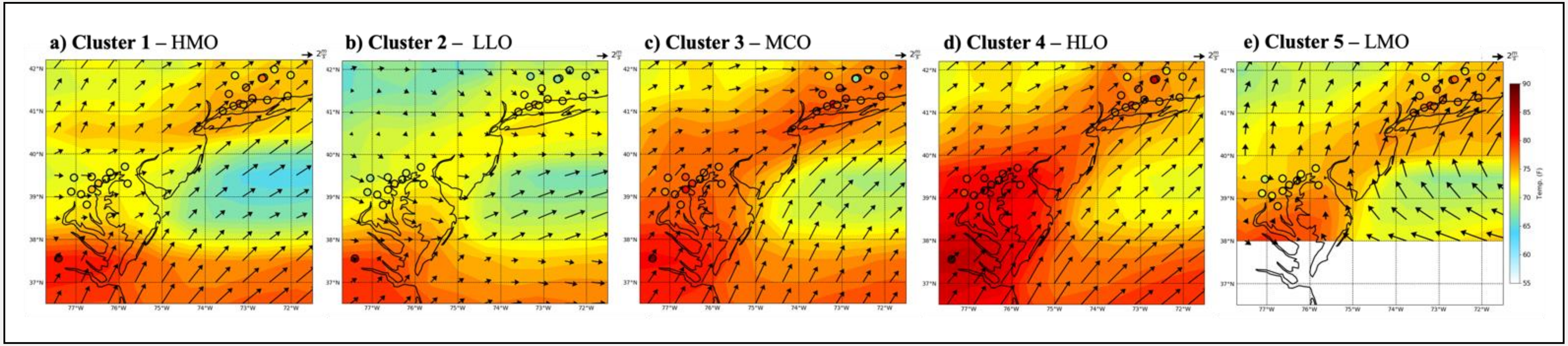


– C1 – C2 – C3 – C4 – C5

Descriptions of clusters:

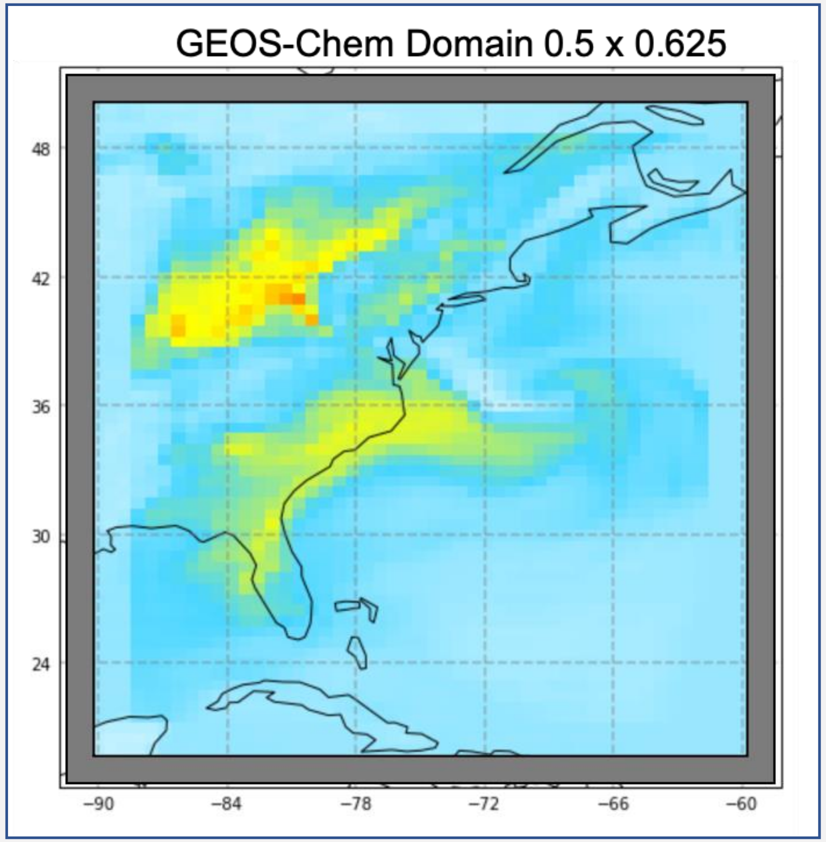
- **Cluster 1** = highest mid-level O_3 (HMO) cluster
- **Cluster 2** = lowest low-level O_3 (LLO) cluster
- **Cluster 3** = most common O_3 (MCO) cluster
- **Cluster 4** = highest low-level O_3 (HLO)
- **Cluster 5** = least common & lowest mid-level O_3 (LMO) cluster

Meteorological surface analyses



- Meteorological conditions support clustered lidar O_3 profiles.
- Cluster 3 & 4 presented higher overall observed & simulated surface temperatures
- Clusters 1, 3, and 4 (highest surface O_3) -- predominant offshore, westerly wind
  - conducive to higher surface O_3 concentrations
- Cluster 2 = lowest temperatures -- cluster with lowest surface O_3 concentrations
- Cluster 5 temperatures moderately high but, in contrast, average wind speed is higher (specific over LIS)
  - wind direction is predominantly onshore (Easterly – Southerly) -- transport of cleaner marine air corroborates lower surface O_3 levels

Model setup



- GEOS-Chem (MERRA2 meteorology) nested 0.5°x 0.625° horizontal resolution ~ using 2°x 2.5° global boundary conditions.
- GEOS Composition Forecasting (GEOS-CF) system 0.25° horizontal resolution data *(https://gmao.gsfc.nasa.gov) (Knowland et al., 2019)*
- Similar chemistry schemes

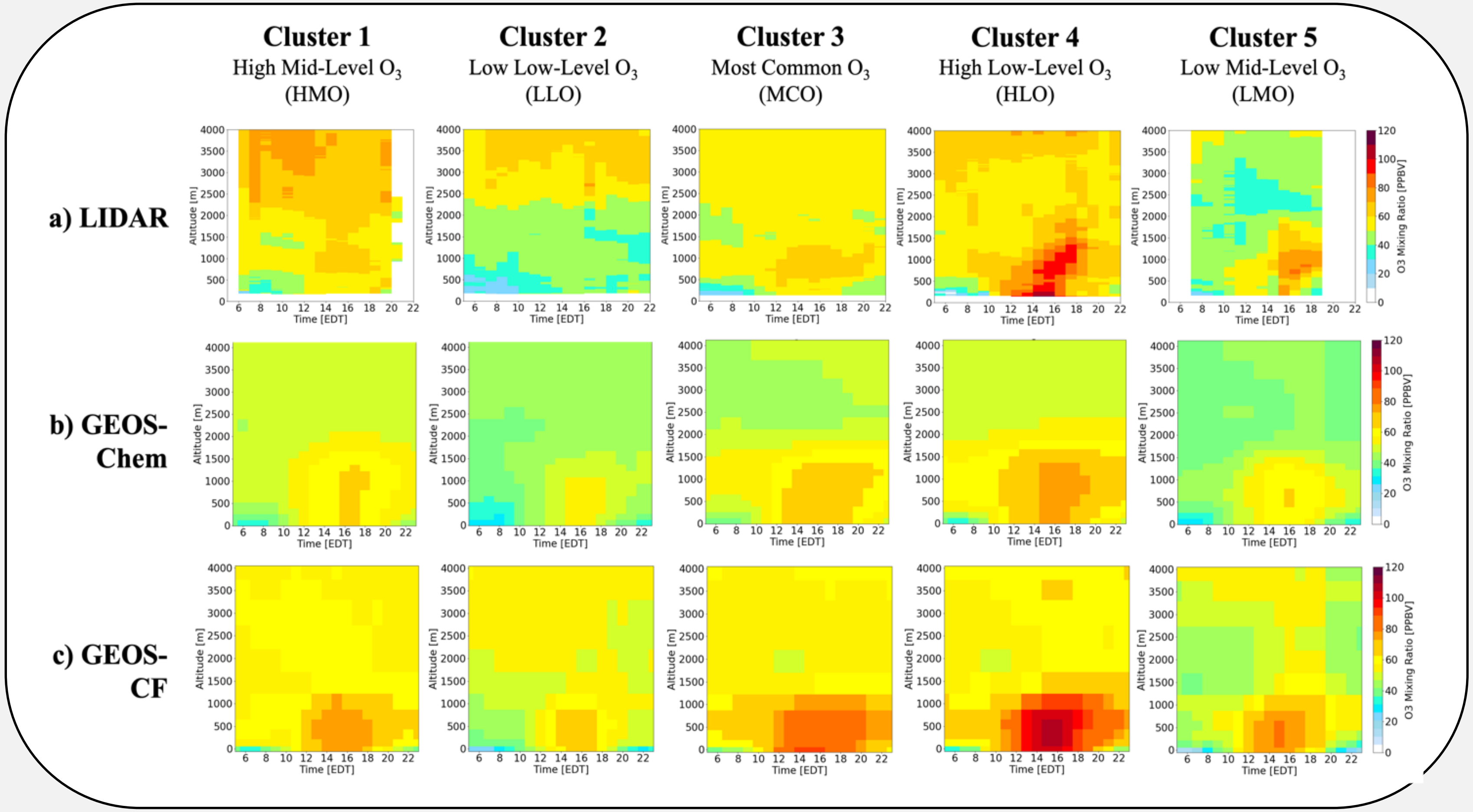
- The main model differences:

1. GEOS-Chem => offline CTM using archived meteorology; GEOS-CF => online, simulates atmospheric composition simultaneously with meteorology
2. GEOS-CF spatial resolution => 0.25°; GEOS-Chem spatial resolution => 0.5° x 0.625°
3. GEOS-CF anthropogenic emissions => Harmonized Gridded Air Pollution (HTAP; v2.2) from the Emission Database for Global Atmospheric Research (EDGAR); GEOS-Chem anthropogenic emissions => CEDS
4. Data only available for <u>2018</u> ~ analysis adjusted for this comparison

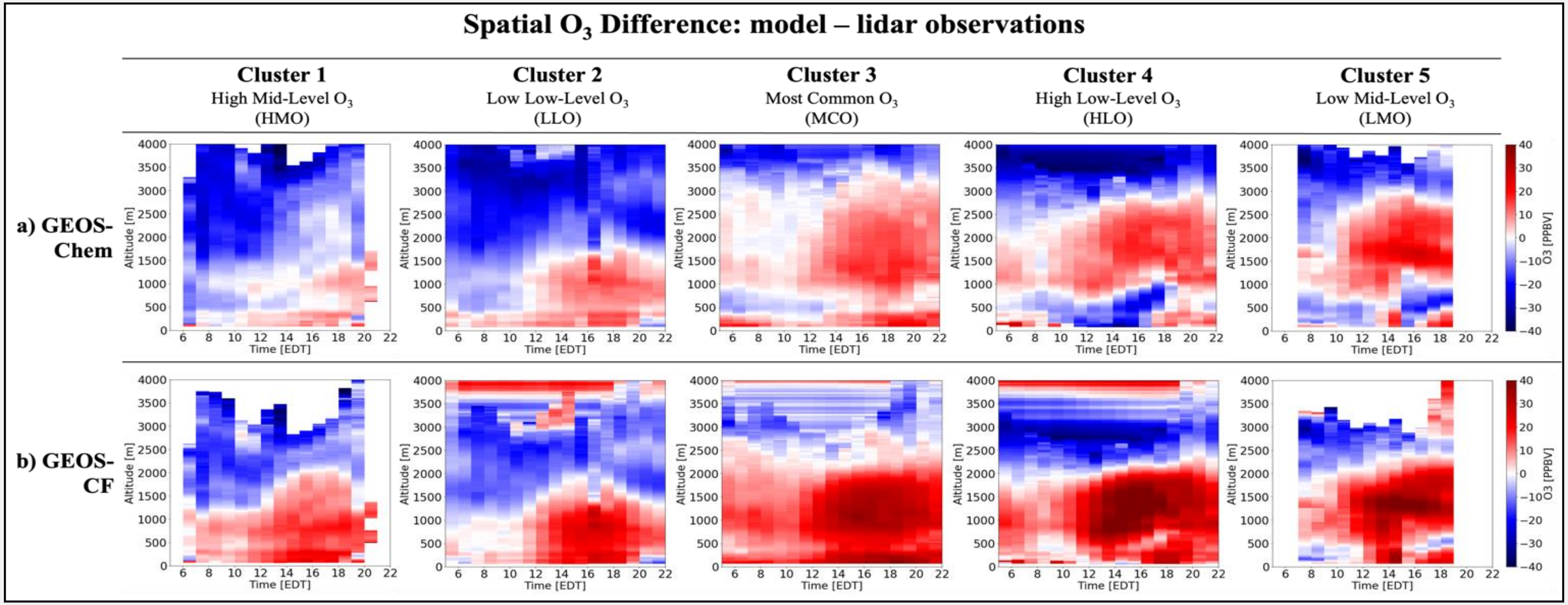
Air Quality Model Results

- Both models simulate low-level O_3 well
- Both models struggle to simulate the magnitude of O_3 in mid-level

- GEOS-Chem simulates low O_3 concentrations best in the low-level altitude (e.g., C2)
- Both models struggled to capture moderately high O_3 in low-level altitudes (e.g., C3)
- Both models underestimate mid-level O_3 with worst performance in C1
- Lower O_3 concentrations are better simulated by both models in mid-level altitudes



Cluster Bias



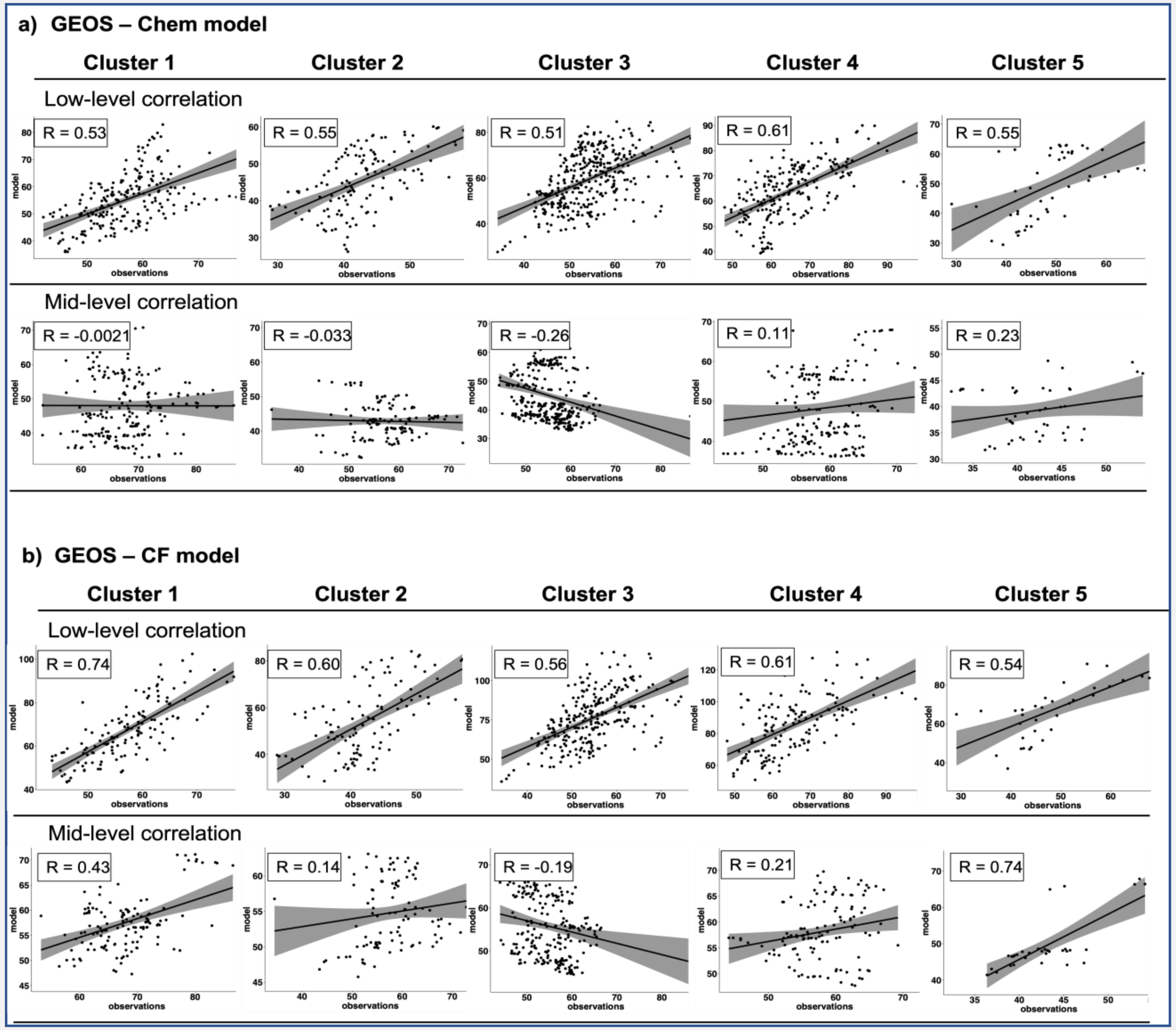
Low-level bias:

- ➢ GEOS-Chem low unsystematic bias range (model – lidar observations)
- ➢ GEOS-CF systematic high **+ bias** but fair relationship

Mid-level bias

- ➢ GEOS-Chem systematic high negative **– bias**
- ➢ GEOS-CF low unsystematic bias

Cluster Bias & Correlation



Bias varies by cluster for both models.

Low-level bias:

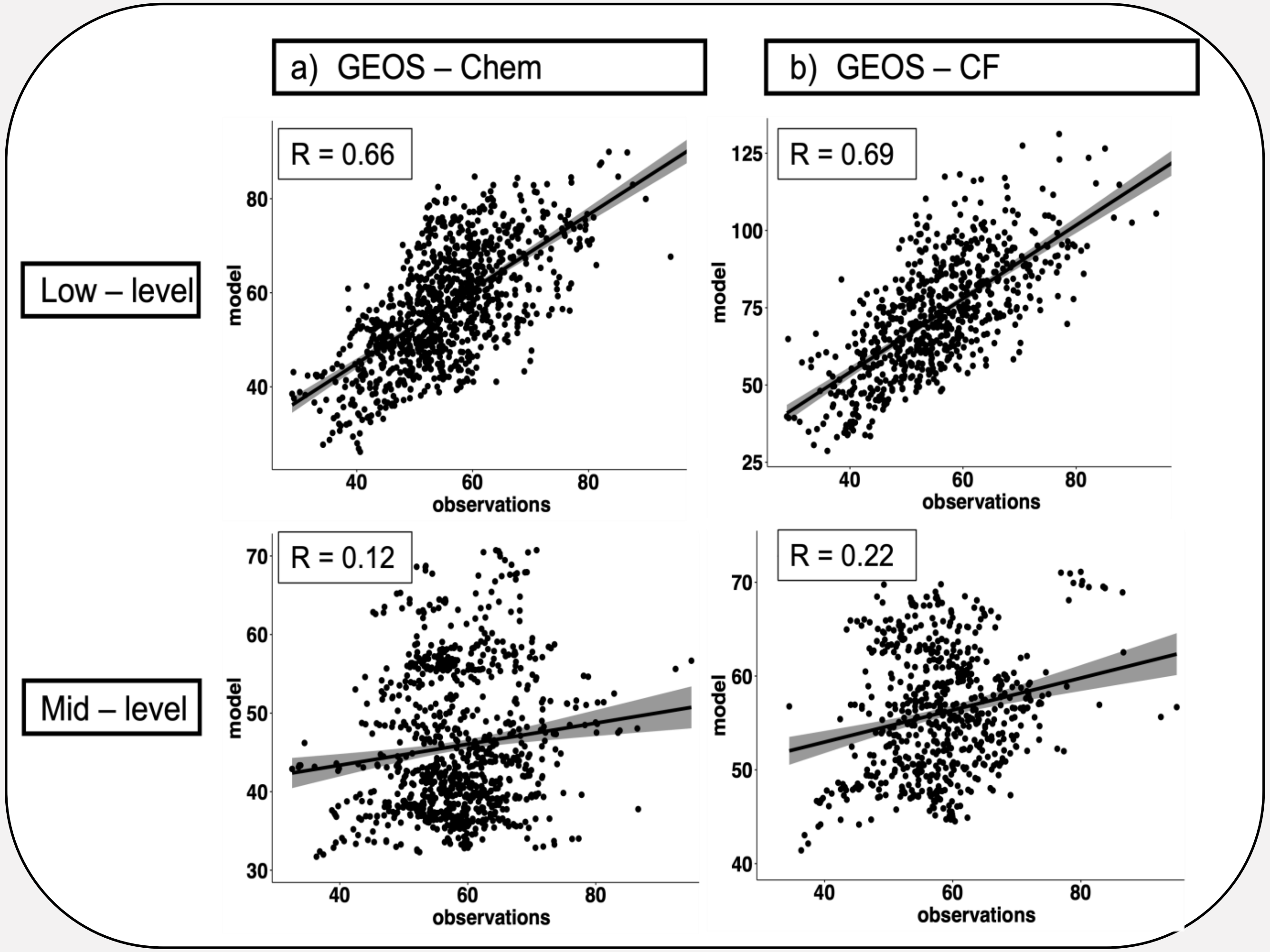
- GEOS-Chem fair relationship with the lidar observations
- Both models able to simulate low-level O_3 pattern well, but GEOS-CF was not able to simulate magnitude consistently overestimating O_3 in low-level altitudes

Mid-level bias:

- GEOS-Chem and GEOS-CF both have a weak relationship with the lidar observations
- Neither simulated mid-level O_3 pattern well, but GEOS-CF was able to simulate magnitude slightly better

Overall Model Correlation

- Overall correlation results indicate GEOS-CF (better grid resolution & an online model) had a slightly better relationship with lidar observations than GEOS-Chem
- There are still limitations to both models especially when simulating mid-level O_3
- Known model errors & coarse horizontal and vertical grid resolution contribute to the difficulty in simulating fine-scale coastal O_3 variability



Impact of meteorological factors on clusters & model performance

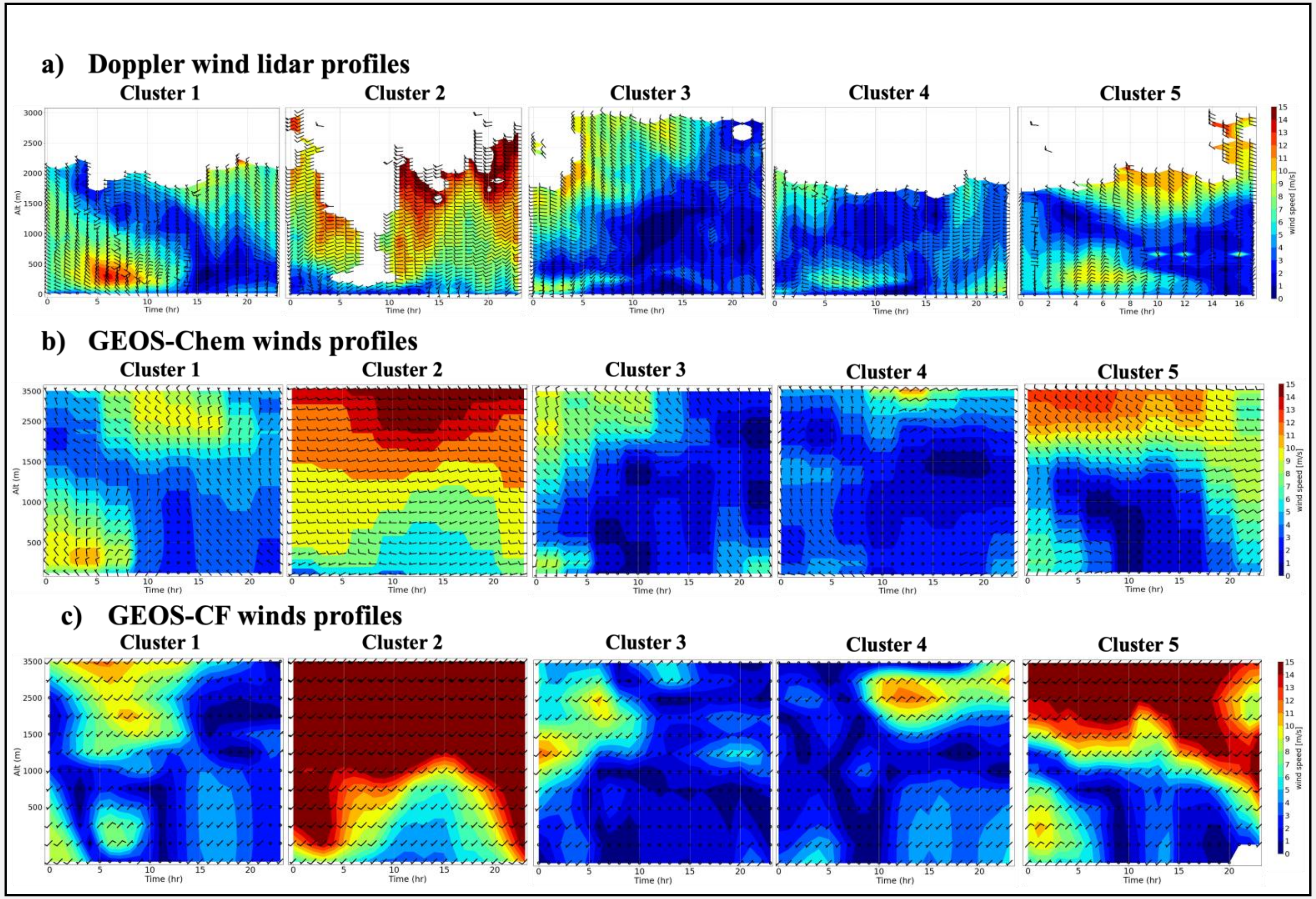
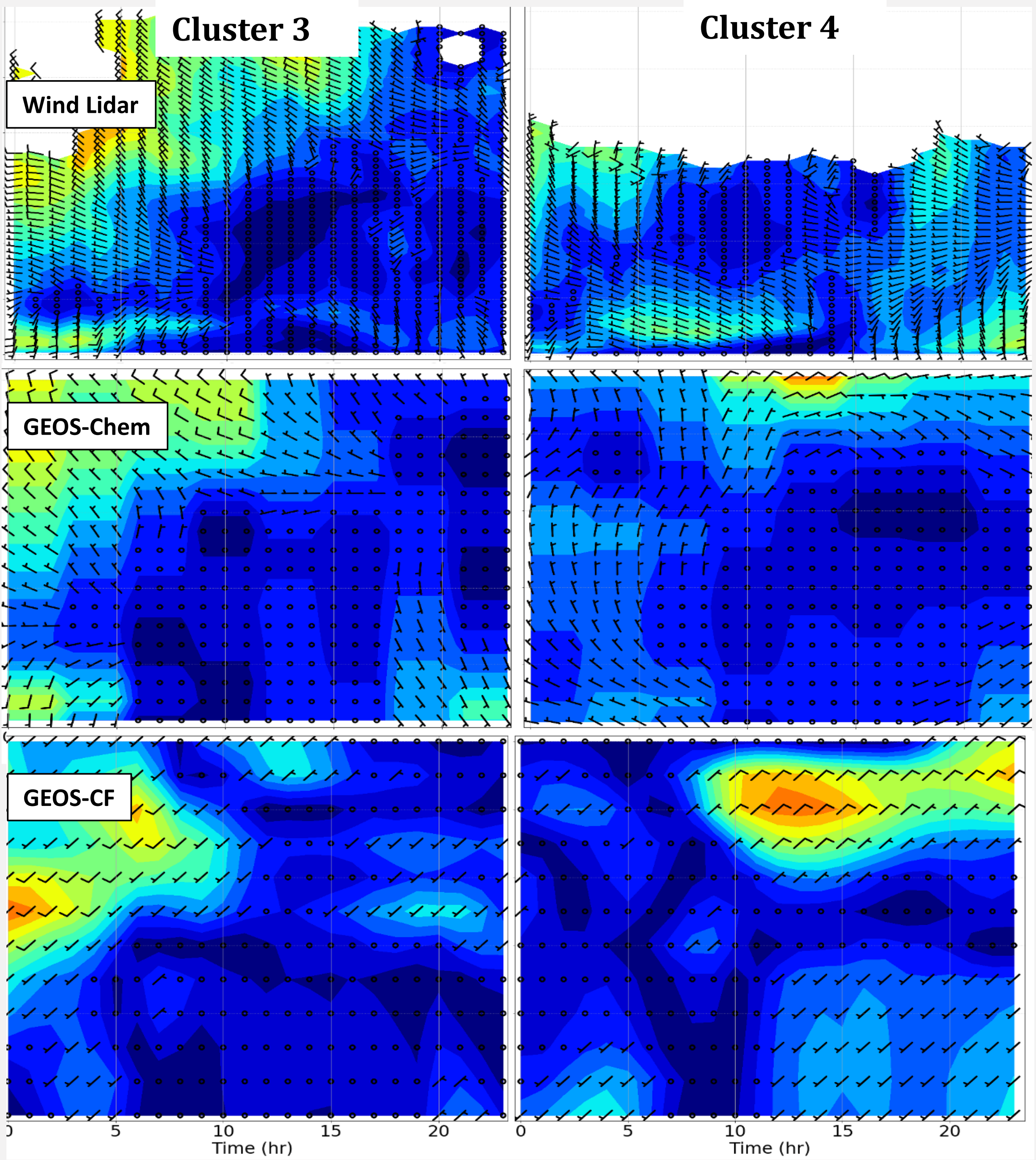


Fig. Vertical profiles of wind speed and direction from a) Doppler wind lidar, b) GEOS-Chem, and c) GEOS-CF model results from OWLETS-2 at HMI. Each figure depicts a date assigned to a specific cluster (1 - 5).

- Wind lidar data mostly limited (< 2000 m)
- Evaluated Doppler wind lidar vs. simulated wind profiles
- General under prediction in windspeeds
- Poorest model performance:
  - Cluster 3 & 4
- Both models had the highest bias & lowest correlation simulating low-level O_3 in <u>*Cluster 3*</u>
- The models struggle to capture the finer processes captured by lidar



Sea Breeze cases

- Midday wind deceleration & directional shift (offshore → onshore) at 11:00 LT accompanied by calm winds (0 m/s)
- Indicating possible common sea/bay breeze event
- Sea breeze events give cause to enhanced surface O_3
- Timing of event poorly simulated
- Models predict little/no wind much earlier in profile (begin at 06:00 LT) & no well-defined shift
- Coarser model resolution = not able to capture phenomena in these cases
- Could have facilitated in high O_3 biases for these clusters

- Although GEOS-CF has a finer horizontal resolution than GEOS-Chem, results do not reveal advantages simulating wind speed/direction
- Affirms GEOS-CF spatial resolution (~25 km) still not fine enough for processes such as the sea/bay breeze

Conclusion

- Clustering approach allowed us to characterize a range of variable vertical & temporal coastal O_3 behavior for the duration of these campaigns
- Can be a good indicator of how O_3 behaves in general in coastal regions during summer months
- Clustering analysis provided an abridged method to evaluate performance of two CTMs, GEOS-Chem & GEOS-CF
- Curated clusters reveal current limitations & cases which CTMs fare simulate coastal O_3 well
- Model simulations struggle to reproduce the O_3 vertical profile magnitude, specifically in the mid-level
- Fine processes (sea/bay breeze) were still difficult to simulate even with grid resolutions …

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Extra:

Clustering application

- Features evaluated for cluster tendency (to confirm dataset contained meaningful clusters)
- Hopkins statistic which measures whether there is uniform distribution (spatial randomness) within dataset (Lawson & Jurs, 1990)
- Results: value higher than 0.75 (actual = 0.77) which by this standard indicates a clustering tendency at the 90% confidence level
- Evaluating different feature options did not lead to better statistical results than with the final chosen features
- *Nbclust* (Charrad et al., 2014) used: applies 30 indices for determining optimal number of clusters
- Tested quality of clustering results using silhouette method (Kaufman & Rousseeuw, 1990)
- Results: 6 clusters – later 5
- K-Means clustering algorithm based on Euclidean distance to each centroid
  - input data normalized (to a mean of zero & standard deviation of one)
  - to ensure each feature is given same importance in clustering (Aksoy & Haralick, 2001; Larose, 2005)

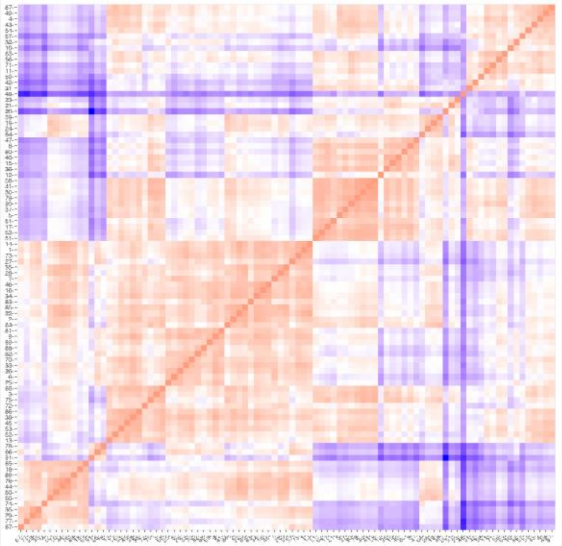

Figure S1. Visual assessment of cluster tendency (VAT) approach. Dataset high similarity (red) and low similarity (blue).

Missing data

- Input features were tailored based on structure of lidar measurements (limitations), remaining data still had missing data points
- Most cases of missing data points:
  - earlier morning measurements (06:00 – 12:00 EDT)
  - later evening measurements (16:00 – 21:00 EDT)
- 51/91 O_3 profile curtains had at least <u>*one*</u> missing data point (feature)
- Complete case analysis (CCA) (e.g. only 40 O_3 curtains)
- Single imputation (SI) technique (*knnImputation)* to fill in missing data
- Allows use of full 91 profile curtains of O_3 data ~ imputated
- Silhouette method used to test quality of newly imputed dataset
- Proved to be no worse, nor better, than CCA (*real data*) results

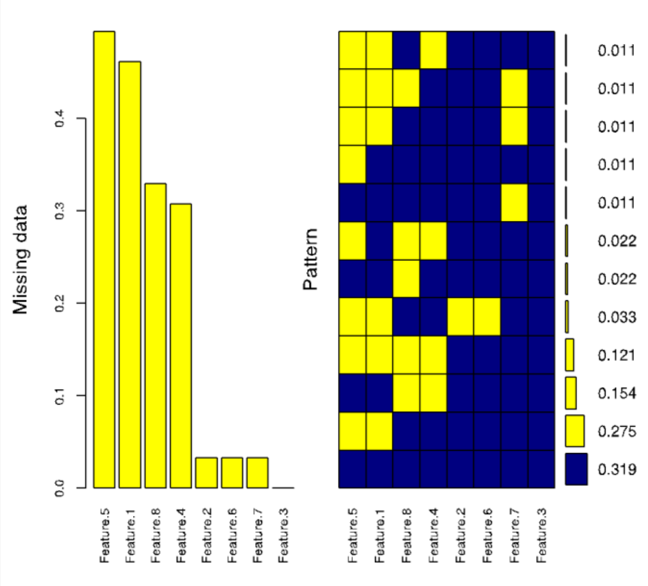

Figure S2. Percentage and pattern of missing data points by each feature used for clustering.